chain nodes :
    13 17 19 20 21 22 23 28 29 30 31 34 35 37 38 46
ring nodes :
    1 2 3 4 5 6 7 8 9 10 11 12 39 40 41 42 43 44
chain bonds :
    4-7 6-19 19-20 20-21 21-22 22-23 28-29 28-30 30-31 34-35 34-37 37-38
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 39-40 39-44 40-41 41-42
    42-43 43-44
exact/norm bonds :
    1-2 1-6 2-3 3-4 4-5 4-7 5-6 6-19 19-20 20-21 21-22 22-23 28-29 28-30 30-31 34-35
    34-37 37-38 39-40 39-44
normalized bonds :
    7-8 7-12 8-9 9-10 10-11 11-12 40-41 41-42 42-43 43-44
isolated ring systems :
    containing 1 : 7 : 39 :

G1:CH3,Et

G2:C,N

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
    12:Atom 13:CLASS 14:Atom 17:CLASS 18:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS
    28:CLASS 29:CLASS 30:CLASS 31:CLASS 33:Atom 34:CLASS 35:CLASS 36:Atom 37:CLASS
    38:CLASS 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:CLASS 47:Atom